# Time Optimal Unitary Operations

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Extending our previous work on time optimal quantum state evolution, we formulate a variational principle for the time optimal unitary operation, which has direct relevance to quantum computation. We demonstrate our method with three examples, i.e. the swap of qubits, the quantum Fourier transform and the entangler gate, by choosing a two-qubit anisotropic Heisenberg model.

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Time optimal quantum computation is attracting a growing attention [1, 2, 3] besides the more conventional concept of optimality in terms of gate complexity, i.e. the number of elementary gates used in a quantum circuit [4]. The minimization of physical time to achieve a given unitary transformation is relevant for the design of fast elementary gates. It also provides a physical ground to describe the complexity of quantum algorithms, whereas gate complexity should be regarded as a more abstract concept in which physics is implicit. Works relevant to the former subject can be found, e.g., in Refs. [1] and [2], which discuss the time optimal generation of unitary operations for a small number of qubits using a Cartan decomposition scheme and assuming that one-qubit operations can be performed arbitrarily fast. An adiabatic solution to the optimal control problem in holonomic quantum computation was given in Ref. [5], while the geometry of the projective unitary group was exploited in Ref. [3] to derive tight upper bounds on the time complexity of certain quantum gates. Nielsen et al. [6] proposed a criterion for optimal quantum computation in terms of a certain geometry in Hamiltonian space, and showed in Ref. [7] that the quantum gate complexity is related to optimal control cost problems. The authors of Ref. [8] suggested a geometrical method for the efficient synthesis of the controlled-NOT gate between two qubits with a special Hamiltonian.

Recently, the authors discussed the quantum brachistochrone for state evolution [9], i.e. the problem of finding the time optimal evolution and the optimal Hamiltonian of a quantum system for given initial and final states. It was formulated as an action principle for the quantum state in the complex projective space endowed with the Fubini-Study metric, and the Hamiltonian subject to certain constraints. We obtained the time optimal state evolution and the optimal Hamiltonian by solving the Euler-Lagrange equations. In this paper we extend the methods used in Ref. [9] and we describe the general framework for finding the time optimal realization of a given unitary operation. Roughly speaking, we replace the projective space representing quantum state vectors with the space of unitary operators. While the optimality in the previous work depends on the initial state, it does not in the present case so that it is more directly relevant to subroutines in quantum computation, where the input may be unknown.

Let us consider the problem of evolving a unitary operator $U(t)$ with Hamiltonian $H(t)$ and of achieving a target unitary operation $U_f$. There must be some constraints for $H(t)$, otherwise one would be able to realize $U_f$ in an arbitrarily short time simply by rescaling the Hamiltonian [9]. Thus at least the ‘magnitude’ of the Hamiltonian must be bounded, and physically this corresponds to the fact that one can afford only a finite energy in the experiment. Besides the normalization constraint, the available Hamiltonians may be subject also to other constraints, which can represent either experimental requirements (e.g., the specifications of the apparatus in use) or theoretical conditions (e.g., allowing no operations involving three or more qubits).

We consider the following action for the dynamical variables $U(t)$ and $H(t)$,

$$S(U, H, \Lambda, \lambda_j) := \int dt\, [L_T + L_S + L_C] \tag{1}$$

with

$$L_T := \sqrt{\frac{\langle \frac{dU}{dt}, (1 - P_U)\,(\frac{dU}{dt})\rangle}{\langle HU, (1 - P_U)(HU)\rangle}}, \tag{2}$$

$$L_S := \langle \Lambda, i\frac{dU}{dt}U^\dagger - H\rangle, \tag{3}$$

$$L_C := \sum_j \lambda_j f^j(H), \tag{4}$$

where $\langle A, B\rangle := \operatorname{Tr} A^\dagger B$ and $P_U(A) := \frac{1}{N}\operatorname{Tr}(AU^\dagger)U$. The Hermitian operator $\Lambda(t)$ and the scalars $\lambda_j(t)$ are Lagrange multipliers. The Lagrangian term $L_T$ gives the time duration and corresponds to $\int \frac{ds}{v}$, where $v$ is the velocity of the particle, in the classical brachistochrone. The metric $ds_U^2 = \langle dU, (1 - P_U)(dU)\rangle$ is analogous to the Fubini-Study metric $ds_{FS}^2 = \langle d\psi|(1 - |\psi\rangle\langle\psi|)|d\psi\rangle$ for the quantum state $|\psi\rangle$ and is invariant under left and right

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global $SU(N)$ multiplications. The variation of $L_S$ by $\Lambda$ gives the Schrödinger equation

$$i\frac{dU}{dt} = HU, \quad \text{or} \quad U(t) = \mathcal{T}e^{-i\int_0^t H dt}, \tag{5}$$

where $\mathcal{T}$ is the time ordered product. This is similar to the case of the quantum brachistochrone for quantum states [9]. The variation of $L_C$ by $\lambda_j$ leads to the constraints for $H$,

$$f_j(H) = 0. \tag{6}$$

It is natural to assume that the constraint functions $f_j(H)$ actually depend only on the traceless part of $H$, i.e. $\widetilde{H} := (1 - P_1)(H) = H - (\operatorname{Tr} H)1/N$. In this case, the action $S$ is invariant under the $U(1)$ gauge transformation $U \mapsto e^{i\theta}U$, $H \mapsto H - \frac{d\theta}{dt}$, $\Lambda \mapsto \Lambda$, $\lambda_j \mapsto \lambda_j$, where $\theta$ is a real function. In the following we will consider the time optimal evolution of operators belonging to the group $U(N)/\,U(1) \simeq SU(N)$. We note here that, when the Hamiltonian is time independent, the unitary operator actually evolves along a geodesic with respect to the metric $ds_U^2$. This can be easily seen from (5), which implies $\frac{d}{dt}\left[(1 - P_1)\left(\frac{dU}{dt}U^\dagger\right)\right] = 0$, the same equation as derived from the variation by $U$ of the arclength $ds_U$.

Let us now derive the other equations of motion. Before taking variations, it is convenient to rewrite $L_T$, using the relation $P_U(A) = P_1(AU^\dagger)U$, as

$$L_T = \sqrt{\frac{\langle \frac{dU}{dt}U^\dagger, (1 - P_1)(\frac{dU}{dt}U^\dagger)\rangle}{\langle H, (1 - P_1)(H)\rangle}}. \tag{7}$$

The variation of $S$ by $H$, upon using (5), gives

$$\Lambda = F - \frac{\widetilde{H}}{\operatorname{Tr}\widetilde{H}^2}, \tag{8}$$

where we have defined

$$F := \frac{\partial L_C}{\partial H}. \tag{9}$$

Let us now take the variation of $S$ by $U$. Noting that, for any $A$, $\operatorname{Tr} A\delta(\dot{U}U^\dagger) = \operatorname{Tr}(\dot{A} + [A, \dot{U}U^\dagger])U\delta U^\dagger$ up to a total time derivative, we obtain, with the help of (5), $i\frac{d\Lambda}{dt} = [H, \Lambda] - i\frac{d}{dt}\left(\frac{\widetilde{H}}{\operatorname{Tr}\widetilde{H}^2}\right)$. Finally, eliminating $\Lambda$ from (8) and the last equation, we obtain the *quantum brachistochrone equation*

$$i\frac{dF}{dt} = [H, F], \quad \text{or} \quad F(t) = U(t)F(0)U^\dagger(t). \tag{10}$$

This, together with the Schrödinger equation (5) and the constraints (6), is our fundamental equation [10]. It seems universal, as it holds also in the case of time optimal evolution of pure [9] and mixed [11] quantum states.

Given a target operation $U_f$, the optimal time duration $T$, the optimal $H$ and the Lagrange multipliers are determined by the condition that, modulo a global $U(1)$ phase $\chi \in \mathbb{R}$,

$$U(T) = e^{i\chi}\, U_f. \tag{11}$$

To solve (10) one should first choose a gauge, and the most natural choice is to take $\widetilde{H} = H$. Then, from (10), together with the constraints (6), one obtains $H$ and, using (5), one finally gets $U$. If we assume that the normalization condition for $H$ has the form

$$f(H) := \tfrac{1}{2}(\operatorname{Tr} H^2 - N\omega^2) = 0, \tag{12}$$

where $\omega$ is a constant, then the constraint part of the Lagrangian can be rewritten as

$$L_C = \lambda f(H) + L'_C, \tag{13}$$

where $\lambda$ is a Lagrange multiplier and $L'_C$ is the sum of the other constraints. Then, from (9) we obtain

$$F = \lambda H + F', \tag{14}$$

where $F' := \frac{\partial L'_C}{\partial H}$.

In many problems in quantum computation or quantum control, the constraints, except the normalization of $H$, are linear and homogeneous, namely,

$$L'_C = \sum_j \lambda_j \operatorname{Tr} g_j H, \tag{15}$$

where $g_j \in su(N)$, and $\lambda_j(t)$ are Lagrange multipliers. Then, from (14) one gets $F' = \sum_j \lambda_j g_j$. Due to (6), $F'$ and $H$ orthogonal,

$$\operatorname{Tr} HF' = 0. \tag{16}$$

It is also easy to show that $\lambda$ in (14) is a constant, and it can be chosen equal to one by a simple rescaling of $F$.

Let us consider as a specific model a physical system which consists of two qubits represented by two spins interacting via controllable, anisotropic couplings $J_k(t)$ ($k = x, y, z$) and subject to local, controllable magnetic fields $B^i(t)$ ($i = 1, 2$) restricted to the $z$-direction. In other words, we choose the following two-qubit Heisenberg Hamiltonian,

$$H := -J_k\sigma_k^1\sigma_k^2 + B^1\sigma_z^1 + B^2\sigma_z^2, \tag{17}$$

where $\sigma_k^1 := \sigma_k \otimes 1$, $\sigma_k^2 := 1 \otimes \sigma_k$ and $\sigma_k$ are the Pauli operators. In the standard computational basis (which we adopt from here on), the Hamiltonian (17) is block diagonal, i.e.

$$H = \begin{bmatrix} -J_z+B_+ & 0 & 0 & -J_- \\ 0 & J_z+B_- & -J_+ & 0 \\ 0 & -J_+ & J_z-B_- & 0 \\ -J_- & 0 & 0 & -J_z-B_+ \end{bmatrix}, \tag{18}$$

where we have introduced $B_\pm(t) := B^1(t) \pm B^2(t)$ and $J_\pm(t) := J_x(t) \pm J_y(t)$. The choice (17) for the physical Hamiltonian is guaranteed by the operator (see (16))

$$F' = \sum_{i\neq j} \lambda_{ij}\sigma_i^1\sigma_j^2 + \xi_1\sigma_x^1 + \xi_2\sigma_x^2 + \eta_1\sigma_y^1 + \eta_2\sigma_y^2, \tag{19}$$

where $\lambda_{ij}(t)$, $\xi_i(t)$ and $\eta_i(t)$ are Lagrange multipliers. The normalization constraint (12) now reads

$$B_+^2 + B_-^2 + J_+^2 + J_-^2 + 2J_z^2 = 2\omega^2. \tag{20}$$

We can thus solve the quantum brachistochrone equation (10) using (14), (17) and (19). After some elementary algebra (by comparing the coefficients of orthogonal generators of $SU(4)$ on both sides of (10)), we find that the Lagrange multipliers $\lambda_{xy}$ and $\lambda_{yx}$ and the coupling $J_z$ are constants. Furthermore, equations for the control variables $B_\pm$ and $J_\pm$ decouple from those for the other variables and we obtain,

$$B_\pm(t) = B_{0\pm}\cos 2(\gamma_\pm t + \psi_\pm), \tag{21}$$
$$J_\pm(t) = \mp B_{0\mp}\sin 2(\gamma_\mp t + \psi_\mp), \tag{22}$$

where $B_{0\pm}, \psi_\pm$ and $\gamma_\pm := \lambda_{xy} \pm \lambda_{yx}$ are constants. Equations (21) and (22) are enough to solve for the optimal $H(t)$ and $U(t)$. In particular, thanks to the block-diagonal form (18) of the Hamiltonian, our task to solve the Schrödinger equation (5) is much simplified and we finally get the optimal unitary evolution operator as

$$U(t) = \begin{bmatrix} e^{iJ_zt}(\alpha_{0+}+i\alpha_{z+}) & 0 & 0 & e^{iJ_zt}(\alpha_{y+}+i\alpha_{x+}) \\ 0 & e^{-iJ_zt}(\alpha_{0-}+i\alpha_{z-}) & e^{-iJ_zt}(\alpha_{y-}+i\alpha_{x-}) & 0 \\ 0 & e^{-iJ_zt}(-\alpha_{y-}+i\alpha_{x-}) & e^{-iJ_zt}(\alpha_{0-}-i\alpha_{z-}) & 0 \\ e^{iJ_zt}(-\alpha_{y+}+i\alpha_{x+}) & 0 & 0 & e^{iJ_zt}(\alpha_{0+}-i\alpha_{z+}) \end{bmatrix}, \tag{23}$$

where we have chosen $U(0) = 1$ and we have introduced

$$\begin{aligned} \alpha_{0\pm}(t) &:= \cos\gamma_\pm t\cos\Omega_\pm t + \tfrac{\gamma_\pm}{\Omega_\pm}\sin\gamma_\pm t\sin\Omega_\pm t, \\ \alpha_{x\pm}(t) &:= \pm\tfrac{B_{0\pm}}{\Omega_\pm}\sin\Omega_\pm t\sin(\gamma_\pm t + 2\psi_\pm), \\ \alpha_{y\pm}(t) &:= \pm(\sin\gamma_\pm t\cos\Omega_\pm t - \tfrac{\gamma_\pm}{\Omega_\pm}\cos\gamma_\pm t\sin\Omega_\pm t), \\ \alpha_{z\pm}(t) &:= -\tfrac{B_{0\pm}}{\Omega_\pm}\sin\Omega_\pm t\cos(\gamma_\pm t + 2\psi_\pm), \end{aligned} \tag{24}$$

with $\alpha_{0\pm}^2 + \boldsymbol{\alpha}_\pm^2 = 1$, and where $\Omega_\pm := \sqrt{B_{0\pm}^2 + \gamma_\pm^2}$.

The next step is to find out the coefficients $J_z, \alpha_{0\pm}(T)$ and $\boldsymbol{\alpha}_\pm(T)$ (i.e. the constants $B_{0\pm}, \gamma_\pm$ and $\psi_\pm$), the time duration $T$ and the global phase $\chi$ which realize the target (11). We now demonstrate this explicitly by a few simple but interesting examples.

*The* SWAP *gate:* Let us assume that our target is the SWAP gate

$$U_{\text{SWAP}} := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{25}$$

which exchanges the states of qubits 1 and 2. Solving (11) by comparison of the matrix elements of (23) and (25) and using (24), we obtain the following set of parameters: $B_{0+} = \gamma_- = 0$, $B_{0-}T = \frac{\pi}{2}(1+2p)$, $J_zT = -\frac{\pi}{4}[1-2(p+q)-4(m-n)]$, $2\psi_- = \frac{\pi}{2}(1+2q)$, and $\chi = -\frac{\pi}{4}[1-2(p+q)+4(m+n)]$, where $m, n, p$ and $q$ are arbitrary integers and $T$ is still to be determined. The zero values of $B_{0+}$ and $\gamma_-$, together with (21) and (22), imply that $B_\pm$ and $J_\pm$ are constants and therefore, via (18), that the optimal Hamiltonian is time independent. The time optimal duration $T_{\text{SWAP}}$ can then be found by imposing the constraint (20), which reads $\left(\frac{4\omega T_{\text{SWAP}}}{\pi}\right)^2 = \min_{m,n,p,q}\{2(1+2p)^2 + [1-2(p+q)-4(m-n)]^2\}$. The solutions are $p = 0$ and $q = -2(m-n)$ (or $q = -2(m-n)+1$), which lead to $\omega T_{\text{SWAP}} = \frac{\sqrt{3}}{4}\pi$ and

$$H = (-1)^q\frac{\omega}{\sqrt{3}}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{26}$$

*The* ‘QFT’ *gate:* Suppose now that we want to realize the slightly modified target operation

$$U_{\text{‘QFT’}} := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & i \end{bmatrix}. \tag{27}$$

This gate is important as it is essentially equivalent to performing a quantum Fourier transform (QFT) over two qubits, i.e. $U_{\text{QFT}} = W_1 U_{\text{‘QFT’}} W_1$, where $W_1$ is the Hadamard transform acting on qubit 1, i.e. $W_1 := \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \otimes 1$ (for the explicit definition of the QFT see [4]). The QFT is at the core of many quantum algorithms, such as the celebrated Shor's algorithm [12] for factoring integers. If we can assume that the Hadamard transform takes negligible time, our methods generate the time optimal Hamiltonian to obtain the target $U_{\text{QFT}}$. An analysis similar to that for the SWAP gate gives the time optimal duration $\omega T_{\text{‘QFT’}} = \frac{\sqrt{11}}{8}\pi$ and the optimal Hamiltonian as

$$H = \frac{\omega}{\sqrt{11}}\begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 \\ 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{28}$$

*The entangler gate:* As a last example, we want to find the optimal way to generate the entangler gate

$$U_{\text{ENT}} := \begin{bmatrix} \cos\varphi & 0 & 0 & \sin\varphi \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sin\varphi & 0 & 0 & \cos\varphi \end{bmatrix}, \tag{29}$$

where we choose the angle $\varphi \in [0, 2\pi]$. This gate, upon acting on the initial state $|00\rangle$, produces the $\varphi$-dependent entangled state $\cos\varphi|00\rangle - \sin\varphi|11\rangle$. For example, when $\varphi = 3\pi/4, \pi/4$, this allows reaching the maximally entangled Bell states $|\Phi^{\pm}\rangle := (|00\rangle \pm |11\rangle)/\sqrt{2}$. As usual, comparison of (23) and (29) gives the optimal, $\varphi$-dependent $\omega T_{\text{ENT}} = \pi\sqrt{x(1-x/2)}$ and

$$H(t) = \pm\sqrt{2}\omega \begin{bmatrix} -\cos\mu(t) & 0 & 0 & \sin\mu(t) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sin\mu(t) & 0 & 0 & \cos\mu(t) \end{bmatrix}, \tag{30}$$

where $\mu(t) := 2(\gamma_+ t + \psi_+)$, $\gamma_+(x) = \omega(x-1)/\sqrt{x(1-x/2)}$ and $x := \varphi/\pi$ (see figure 1).

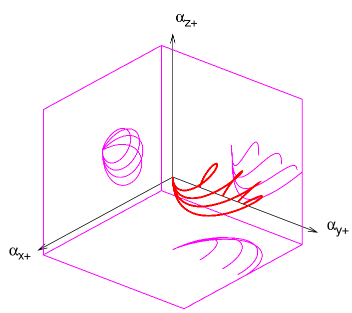


FIG. 1: Curves for the unitary evolutions (23) of the entangler gate with $\varphi = \frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}$ and $\frac{\pi}{2}$, with projections on the $\boldsymbol{\alpha}_+$ planes. Geodesics from the origin would be straight lines.

To summarize, we have studied the problem of finding the time optimal evolution of a unitary operator in $SU(N)$ and the corresponding time optimal Hamiltonian within the context of a variational principle. This is a natural extension of our previous analysis of the time optimal evolution of quantum states in the projective space, and it may be of greater relevance for quantum computation, whereas the task of finding the best quantum algorithm achieving a certain final answer can be mapped to the problem of finding the best sequence of unitary operations with respect to some cost function (time) subject to certain physical or theoretical constraints. In particular, we explicitly found the optimal Hamiltonian and the optimal duration for three important examples of quantum gates acting on two qubits. The optimal Hamiltonians realizing the SWAP and QFT gates are time independent and, therefore, the corresponding optimal unitary operators follow geodesic curves on the $SU(4)$ manifold endowed with the metric $ds_U^2$. This is not the case for the entangler gate, and as one may expect for the case of generic gates, where the optimal Hamiltonian is time dependent and the time evolution of the corresponding unitary operator is not geodesic. We should caution the reader that, in order to make the variational principle well defined, the action (1) should be actually expressed as an integration over a parameter with fixed initial and final values. Since this does not affect our results, we have omitted these details for simplicity. Furthermore, we note that, instead of (2), any function of $i\dot{U}U^\dagger$ and $H$ which becomes constant upon using the Schrödinger equation would produce the same quantum brachistochrone equation (10). In this sense, the choice of the metric in (2) is not essential for our formulation. Finally, as for further developments, we do not see any major obstacle in generalizing our models to the case of a higher number of qubits.

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